Accelerating Chemicals Innovation

Molecular Modeling and Artificial Intelligence for a More Efficient R&D

The Spanish computational chemistry start-up Nextmol (Bytelab Solutions), a spin-off from the Barcelona Supercomputing Centre, offers a software-as-a-service (SaaS) platform that accelerates research and innovation in sustainable specialty chemicals through "in silico" experiments using molecular modeling and artificial intelligence (AI). Its cloud-based lab enables molecules and formulations to be characterized directly on the computer, reducing the time and cost of chemical research and development by a factor of five. In an interview with CHEManager, Nextmol's CEO Monica de Mier and Scientific Director Stephan Mohr talk about their revolutionary technology for the specialty chemicals industry.

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Monica de Mier, CEO, and Stephan Mohr, Scientific Director, Nextmol

CHEManager: What was the starting point and motivation for founding Nextmol?

Monica de Mier: The motivation for founding Nextmol was to help the chemical industry in its green and digital transition. With our solutions, we enable a faster development of sustainable chemicals to meet Green Deal goals, comply with environmental regulatory frameworks, and fulfill current consumer demands. We also help in the digitalization of industry by democratizing the use of computational approaches to companies of all sizes through an easy-to-use platform in the cloud. The final purpose is to contribute to the development of safer and more sustainable chemicals for society.

What problem does Nextmol's technology specifically solve, or what previously untapped opportunities does it open up?

Stephan Mohr: Nextmol's technology solves the problem of the long and costly R&D processes in the experimental laboratory. Chemical research is based on a trial-and-error approach that requires a large number of tests before arriving at the molecule with the desired properties.

Nextmol's platform is a computational laboratory to characterize chemical molecules directly on the computer, without synthesizing them. Molecular modeling simulations allow to investigate the behavior of molecular systems on an atomistic level, and to study the fundamental interactions that govern them. These simulations are complemented with data-driven approaches, in particular machine learning, which characterize the molecules solely based on their molecular structure and are therefore well suited to quickly analyze thousands of possible new candidate chemistries. Both techniques can be used to predict the performance of molecules and rank them, and are already being successfully used for the computational study and design of chemicals in many fields.

Who are your customers and in which markets do you find them?

M. de Mier: Our customers are specialty chemicals companies with R&D activities, from chemical majors to SMEs and CDMOs. The platform is best suited for polymer and surfactant chemistries, and allows to study numerous properties and phenomena such as the characterization of biobased polymers and polymer blends, additive migration, adsorption affinity at surfaces / interfaces, synergistic and antagonistic effects, or collective effects — like anti-agglomeration, dispersion, friction reduction — of formulations.

How has the response from the industry been so far?

S. Mohr: The chemical industry is aware of its sustainability and competitiveness challenges, and the transformations that need to be undertaken. For example, we see that the chemical industry unfortunately lags behind in the digitalization of the data they produce in the laboratory. It is urgent to start generating and storing molecular data in a format that can be later leveraged by data-driven approaches.

Our platform is having a very good response from industry as it makes it possible to characterize a large amount of molecules and formulations at a much lower cost than in the experimental laboratory, automates the trial-and-error stage, and identifies the most promising molecules that have certain physico-chemical properties. In this way, our platform guides and complements the experimental work, making the innovation process much more efficient. We go hand in hand with our customers to ensure a successful integration of our platform in their R&D operations.

What will be the next key steps in the development of the company?

M. de Mier: The next steps are to launch new features of the platform, such as our polymer builder, predictive machine learning models for polymer properties, or high-throughput screening capabilities. We are rapidly increasing the complexity of the molecules, formulations, and applications that the platform can solve. Our goal is to be the trusted computational partner of all chemical companies developing polymers and surfactants.

Personal Profile

Monica de Mier is co-founder and CEO of Nextmol. She holds a Bachelor in Mathematics, MSc in Computational Mechanics, PhD in Engineering, and a Master in Business Administration. She has over 15 years of experience in helping organizations in the adoption of computational techniques in their R&D.

Stephan Mohr is co-founder and Scientific Director of Nextmol. He holds a MSc and PhD in Physics (University of Basel, Switzerland). Postdoc at CEA Grenoble (France) and Barcelona Supercomputing Center (Spain). He has large experience in atomistic modelling (molecular dynamics and DFT), algorithmic development, scientific programming, and high-performance computing.

Business Idea

Towards a Digital Chemical R&D

Nextmol's platform is a computational laboratory to characterize chemical molecules directly on the computer (i.e. without having to synthesize them) and thus obtain deep insights about the behavior and mode of action of the molecules. It makes it straightforward to reproduce conditions that are hard to reach experimentally (such as high pressures or temperatures). The platform offers the end-to-end computational characterization of molecules: from the creation of the molecule(s) to study, building of the system, using predefined workflows or creating new ones, running calculations, and analyzing the results. Its main features are summarized here:

- Modeling and calculation of numerous physico-chemical processes and descriptors such as adsorption, agglomeration, surface tension, interfacial tension, glass transition temperature, radius of gyration, persistence length, solubility, and density, among others;
- Modeling based on molecular dynamics;
- Several force fields available;
- Construction of homopolymers and copolymers (block, random) of any size, ionic, branched, cross-linked;
- Wide range of thermodynamic conditions;
- Calculations run in the cloud with the latest GPU hardware;
- Computations can be conducted by non-expert users in computational chemistry;
- Catalog of ready-to-use molecules and workflows;
- Especially suited for polymer and surfactant chemistries.

High-throughput calculations generate large datasets of accurate and consistent results that can be used to train ML models for the fast prediction of properties. Nextmol offers access to ML models for the prediction of, for instance, glass transition temperature (Tg) and solubility parameters of polymers (including biopolymers).

Its computational lab can characterize complex formulations of polymers and surfactants, composed of several million atoms. Furthermore, our technology allows to study a wide range of surface and interface phenomena, such as adsorption affinity at interfaces, formation of self-assembled surface films and micelles, collective effects of adsorbed molecules (dispersion, anti-agglomeration, detergency, etc.), competition for the surface, or synergistic / antagonistic effects.

- Nextmol (Bytelab Solutions), Barcelona, Spain
- https://www.nextmol.com/

NEXTMOL

Elevator Pitch

Computational Chemistry

Nextmol is a deep tech startup dedicated to the development of advanced molecular modeling and artificial intelligence tools to accelerate R&D in the chemical industry. It is a spin-off company of the Barcelona Supercomputing Center, the national supercomputing facility in Spain.

Since its creation in 2019, Nextmol has done projects for several multinational companies, both in the form of services and via its software-as-a-service (SaaS) platform for molecular characterization, and has been granted numerous prestigious national and international grants and awards.

Nextmol is an R&D-intensive company, with a total of 40 years of research experience and more than 60 peer-reviewed publications in high-impact journals among its team members. The company's scientific activity focuses on the development of algorithms and tools for the design of best-in-class and more sustainable chemicals for different applications, including oilfield chemicals, fuel additives, lubricants, detergents, or cosmetics.

Nextmol's mission is to help the chemical industry in its green and digital transition by making the R&D processes much faster and more efficient.

Milestones

2017 – 2019
- Industrial projects at the Barcelona Supercomputing Center

2019
- Creation of Nextmol

2021
- Developed capabilities for surfactants modeling

2022
- South Summit award to Best Industry 5.0 start-up

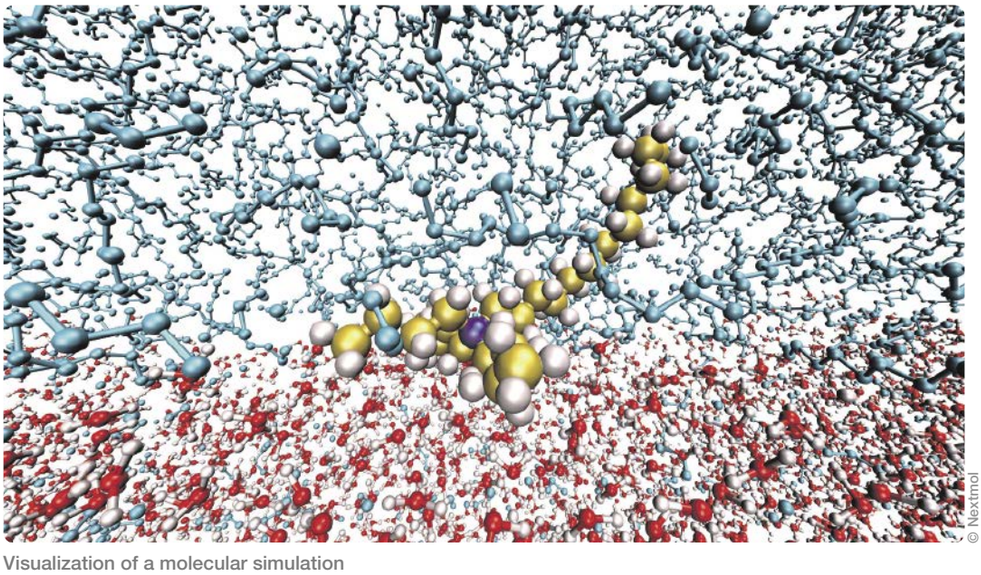
2023
- Carried out successful high-throughput screening of bio-based polymers
- Software platform launched

Roadmap

2024
- Advanced Polymer builder and predictive ML models for polymer properties

2025
- Expansion to new geographies

2026
- Safety and sustainability features



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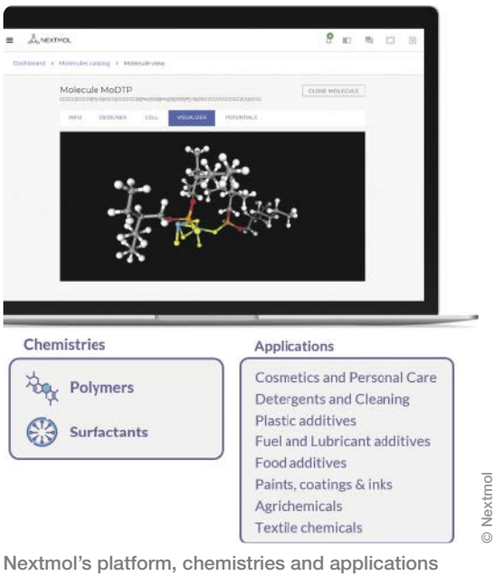
Visualization of a molecular simulation



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Nextmol's platform, chemistries and applications